In-situ Studies of OPV Film Formation: Accelerating the Transition from Lab to Fab

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Solution processing of electrically active layers is a promising route to sustainable manufacturing of functional components on diverse substrates such as flexible foils and textiles. Typically, solution processing does not result in the thermodynamic equilibrium form; instead metastable, kinetically trapped structures dominate. This allows great flexibility in the ability to tailor film structure (and performance) by processing details. The sensitivity of structure and performance to processing is clearly manifest in the fabrication of bulk heterojunction (BHJ) active layers for organic photovoltaics. Organic photovoltaic devices are a promising route to lower costs via roll-to-roll manufacturing. In a BHJ, nano-scale phase separation into nominally bicontinuous donor and acceptor rich regions enables both exciton dissociation and charge extraction. The performance of BHJ based devices is a strong function of the active layer structure and the optimized device structure is, in general, not the equilibrium structure. Recently it has become common to optimize BHJ film formation by introducing small amounts of processing additives. However, the mechanisms by which these additives effect the film formation are not known. We present results from the use of labscale photon based techniques, such as spectroscopic ellipsometry and photoluminescence and synchrotron based grazing incidence x-ray scattering (both wide angle and small angle) on the time evolution of films cast by blade coating, a material conservative model for scalable manufacturing processes. The in-situ measurements provide detailed insights into film thickness, composition, and microstructure. We will discuss highlights from studies of the additive effect in film formation of both polymer and small molecule based BHJs. Multiple mechanisms are revealed with common themes related to control of aggregation through solvent quality and control of growth kinetics via plasticization. We observe that, when elevated solution temperatures are required, significant differences between spin coating and isothermal deposition such as blade coating can arise. We demonstrate that isothermal blade coating is an excellent prototyping tool for slot-die coating by establishing comparable morphologies for small piece blade coating and continuous web slot-die coating.